Theta Vacua, QCD Sum Rules, and the Neutron Electric Dipole Moment

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Abstract

We present a detailed study of the electric dipole moment of the neutron induced by a vacuum theta angle within the framework of QCD sum rules. At next-to-next-to leading order in the operator product expansion, we find the result $d_n(\theta) = 2.4 \times 10^{-16}\bar{\theta}e \cdot cm$, to approximately 40% precision. With the current experimental bound this translates into a limit on the theta parameter of $|\bar{\theta}| < 3 \times 10^{-10}$. We compare this result with the long-standing estimates obtained within chiral perturbation theory, and observe a numerical similarity, but also significant differences in the source of the dominant contribution.

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I. INTRODUCTION

Electromagnetic observables which are odd under T transformations are an important source of information about CP properties of the physics at and above the electroweak scale, complementary to that coming from K and B meson physics. In particular, there are now impressive experimental limits on the electric dipole moments (EDMs) of neutrons, heavy atoms, and molecules [1, 2, 3, 4, 5]. The Kobayashi-Maskawa model, so successful in explaining the observed CP violation in K mesons, predicts EDMs to be several orders of magnitude smaller than the current experimental sensitivity. This presents a unique opportunity for limiting extra sources of CP-violation, and the constraints resulting from EDM data are generally very strong [6].

In principle, EDMs can be used to probe the physics at a high energy scale by limiting the coefficients of operators $\mathcal{O}_i$ with dimension $k \geq 4$ in the effective low energy Lagrangian. The effective Lagrangian for these operators has the form,

$$\mathcal{L} \sim \sum_i c_i M^{4-k} \mathcal{O}_i^{(k)}, \tag{1}$$

where M is the mass scale at which these effective operators are induced and c_i their coefficients which, in general, have logarithmic scale dependence. These operators are odd under CP transformations and their coefficients c_i are proportional to fundamental CP-violating phases of the underlying theory.

Of these contributions, the electron EDM operator is the only example which may be constrained while avoiding the uncertainties necessarily associated with strong interactions. For the EDM of the neutron and the ^{199}Hg atom, many more operators provide important contributions [7, 8, 9, 10, 11]. Particular operators of interest include schematically,

$$G\tilde{G}, \quad \frac{1}{M}\overline{q}F\sigma\gamma_5 q, \quad \frac{1}{M}\overline{q}G\sigma\gamma_5 q, \quad \frac{1}{M^2}GG\tilde{G}, \quad \frac{1}{M^2}\overline{q}\Gamma_1 q\overline{q}\Gamma_2 q, \quad \text{etc.}, \tag{2}$$

where F, G and q stand for electromagnetic, gluon and light quark fields, and $\Gamma_{1,2}$ denotes various contributing matrix structures [8].

In principle, the experiments [1, 2, 3] impose strong constraints on the coefficients c_i. However, in practice, while the operators can be perturbatively evolved down to a scale of order 1 GeV, the ultimate connection between high energy parameters and low energy EDM observables necessarily involves non-perturbative physics. It is this final link which we wish to consider in this paper. The connection between different EDM observables and the coefficients c_i are especially important in supersymmetric theories where the number of relevant operators is much smaller than in a generic scenario and c_i can be explicitly calculated as a function of fundamental CP-violating SUSY phases (For a recent discussion in the context of the MSSM, see e.g. [12]).

In the present paper, we focus on the first of these contributions, $G\tilde{G}$. This has a distinct status in that it has dimension=4 and thus receives contributions at tree-level from the fundamental QCD vacuum angle θ, the parameter labeling different super-selection sectors for the QCD vacuum. Experimental tests of CP symmetry suggest that θ is small and, among different CP-violating observables, the EDM of the neutron $(d_n(\theta))$ is the most sensitive to its value [1, 2]. However, the calculation of $d_n(\theta)$ is a long standing problem [13, 14]. According to Ref. [14], an estimate can be obtained within chiral perturbation

theory, relying on the numerical dominance of a one–loop diagram proportional to $\ln m_\pi$ near the chiral limit. The result can be conveniently expressed in the form

$$d_n = e\theta \frac{m_u m_d}{f_\pi^2(m_u + m_d)} \left(\frac{0.9}{4\pi^2} \ln \frac{\Lambda}{m_\pi} + c \right) \tag{3}$$

and is seemingly justified near the chiral limit where the logarithmic term may dominate over other possible contributions parametrized in this formula by the constant c. However, these incalculable non-logarithmic contributions, can in principle be numerically more important than the logarithmic piece away from the chiral limit. In fact it is also worth noting that in the limit m_u, $m_d \to 0$, the logarithm is still finite, and stabilized, for example, by the electromagnetic mass difference between the proton and neutron. Consequently, one is unable to estimate the uncertainty of the prediction [14]. We note in passing that there is actually an additional $O(1)$ prefactor $(1 - m_\pi^2/m_\eta^2)$ associated with the vanishing of the $U(1)$ anomaly at large N_c, which will play a role subsequently. The explicit derivation of this factor will be given in this paper.

If the logarithm is cut off at the neutron mass, $\Lambda \sim m_n$, and the non-logarithmic terms are ignored, one can derive a bound on the value of θ using the current experimental results on the EDM of the neutron [1, 2]: $\bar{\theta} < O(10^{-10})$. Confronted with a naive expectation of $\theta \sim 1$, the experimental evidence for a small if not zero value for θ constitutes a serious fine tuning dilemma, usually referred to as the strong CP problem. As a consequence, one is usually led to introduce some mechanism via which the primary source of θ, the fundamental vacuum angle, is removed. However, even if this can be achieved, additional corrections are induced via the integration over heavy fields. Within this framework there are two main motivations for refining the calculation of $d_n(\theta)$.

The first refers to theories where the axion mechanism is absent and the θ–parameter is zero at tree level as a result of exact P or CP symmetries [15, 16]. At a certain mass scale these symmetries are spontaneously broken and a nonzero θ is induced through radiative corrections. At low energies, a radiatively induced theta term is the main source for the EDM of the neutron as other, higher dimensional, operators are negligibly small. As θ itself can be reliably calculated when the model is specified, the main uncertainty in predicting the EDM comes from the calculation of $d_n(\theta)$.

The second, and perhaps overriding, incentive to refine the calculation of $d_n(\theta)$ is due to efforts to limit CP-violating phases in supersymmetric theories in general, and in the Minimal Supersymmetric Standard Model (MSSM) in particular. Substantial CP-violating SUSY phases contribute significantly to θ and therefore these models apparently require the existence of the axion mechanism. However, as mentioned above, this does not mean that the θ-parameter is identically zero. While removing $\theta \sim 1$, the axion vacuum will adjust itself to the minimum dictated by the presence of higher dimensional CP-violating operators which generate terms in the axionic potential linear in θ. This induced θ–parameter is then given by:

$$\theta_{induced} = -\frac{K_1}{|K|}, \quad \text{where} \quad K_1 = i \left\{ \int dx e^{iqx} \langle 0|T(\frac{\alpha_s}{8\pi} G\tilde{G}(x), \mathcal{O}_{CP}(0)|0\rangle \right\}_{q=0},$$

where $\mathcal{O}_{CP}(0)$ can be any CP-violating operator with dim>4 composed from quark and gluon fields (as in (2)), while

$$K = i \left\{ \int dx e^{iqx} \langle 0|T(\frac{\alpha_s}{8\pi} G\tilde{G}(x), \frac{\alpha_s}{8\pi} G\tilde{G}(0))|0\rangle \right\}_{q=0} \tag{4}$$

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is the topological susceptibility correlator. In the case of the MSSM, the most important operators of this kind are colour electric dipole moments of light quarks $\bar{q}t^a G^a_{\mu\nu}\sigma_{\mu\nu}\gamma_5 q$, and three-gluon CP-violating operators. The topological susceptibility correlator K was calculated in [17, 18] and the value of θ generated by color EDMs can be found in a similar way [19]. Numerically, the contribution to the neutron EDM, arising from $\theta_{induced}$ is of the same order as direct contributions mediated by these operators and by the EDMs of quarks. Therefore, the complete calculation of d_n as a function of the SUSY CP-violating phases must include a $d_n(\theta)$ contribution and a computation of this value, beyond the logarithmic estimate (3), is needed.

In this paper, we present a detailed application of the QCD sum rule method [20] to obtain an estimate for $d_n(\theta)$ beyond chiral perturbation theory. Within currently available analytic techniques, QCD sum rules seems the most promising approach to this problem as it has, in particular, been used successfully in the calculation of certain baryonic electromagnetic form factors [21, 22]. Within the sum rule formalism, physical properties of the hadronic resonances are expressed via a combination of perturbative and nonperturbative contributions, the latter parametrized in terms of vacuum quark and gluon condensates. We note that previously QCD sum rules were used to estimate the neutron EDM induced by a CP-odd color electric dipole moment of quarks [8, 23]. Surprisingly, these results give d_n $\sim$ 20 times smaller than the estimates based on the chiral loop approach [10]. The calculation of $d_n(\theta)$ using QCD sum rules will certainly help to resolve this controversy. This question is of great numerical importance for the MSSM where color EDMs of quarks are large.

The approach we shall use follows recent work [24] on the θ-induced ρ–meson EDM in reducing the operator product expansion to a set of vacuum condensates taken in an electromagnetic and topologically nontrivial background. Expansion to first order in θ results in the appearance of matrix elements which can be calculated via the use of current algebra [17, 18]. In this approach the θ–dependence naturally arises with the correct quark mass dependence, and the relation to the U(1) problem becomes explicit as $d_n(\theta)$ vanishes when the mass of the U(1) "Goldstone boson" is set equal to the mass of pion.

The initial results from this study were presented in [25], and in this paper we shall present the details of this analysis. We also consider the relation of this result to the estimate (3) obtained within chiral perturbation theory, and compare it with the outcome of an independent calculation of $d_n(\theta)$ reported recently in Ref. [26]. We begin in Section II by studying the phenomenological structure of the neutron correlator, and in particular addressing the issue of how to ensure chiral invariance of the result. In Section III we perform a tree level OPE analysis of the correlator to next-to-next-to leading order which corresponds to sensitivity at the level of $O(1/q^2)$ terms. This requires an investigation of mixing with an additional set of currents CP-conjugate to the usual neutron interpolators. In Section IV, we combine the results of the previous two sections to construct a sum rule for $d_n(\theta)$ which we analyze numerically and extract the estimate,

$$d_n(\theta) = 2.4 \pm 1.0 \times 10^{-16}\bar{\theta}e \cdot cm. \qquad (5)$$

In section V we turn to chiral perturbation theory, and demonstrate explicitly the m^2_η–dependence of the EDM and the CP-odd pion-nucleon coupling constant, indicating their explicit connection to the $U(1)$ problem. We use this result to analyze and contrast the large N_c behavior of the chiral logarithm estimate and the QCD sum rule calculation of the EDM. We point out that, although unimportant numerically, the two results differ in the

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large N_c limit, with the chiral estimate suppressed by a relative factor of $O(1/N_c)$. We then conclude in Section VI with some additional remarks.

II. PHENOMENOLOGICAL PARAMETRIZATION AND CHIRAL INVARIANCE

The starting point for the calculation is the correlator of currents $\eta_n(x)$ with quantum numbers of the neutron in a background with nonzero θ and an electromagnetic field $F_{\mu\nu}$,

$$\Pi(Q^2) = i \int d^4x e^{iq\cdot x} \langle 0|T\{\eta_n(x)\overline{\eta}_n(0)\}|0\rangle_{\theta,F}, \tag{6}$$

where $Q^2 = -q^2$, with q the current momentum.

Before turning to the OPE analysis of this correlator, it is convenient to select an appropriate Lorentz structure to consider and, in the present context, an important criterion will be invariance under chiral rotations. It is crucial to consider this issue when CP-symmetry is broken by a generic quark-gluon CP-violating source – the θ–term in our case – as the coupling between the physical state (neutron) described by a spinor v and the current η_n then acquires an additional phase factor

$$\langle 0|\eta_n|N\rangle = \lambda U_\alpha v, \qquad U_\alpha = e^{i\alpha\gamma_5/2}. \tag{7}$$

The existence of this unphysical phase α is already apparent when one considers the sum rule for the neutron mass, which in the absence of CP-invariance can have an additional Dirac structure proportional to $i\gamma_5$. When we turn to electromagnetic form factors, this angle can mix electric (d) and magnetic (μ) dipole moment structures and complicate the extraction of d from the sum rule.

To see how this will work, we recall that when considering Π in the presence of some external field the phenomenological side of the sum rule may be parametrised by considering the form-factor Lagrangian which encodes the effective (in our case CP violating) vertices (see Fig. 1). We recall that after expanding to leading order in the background field, Π is effectively a three-point correlator, and thus, although one can certainly write a two variable dispersion relation [21], it lacks the powerful positivity constraints which follow from the analytic structure of the two–point correlator. Therefore, its more appropriate to instead explicitly parametrise Π itself, rather than its discontinuity. The corresponding form-factor Lagrangian has the form $\mathcal{L} = \sum_n f_n S(q)\mathcal{O}_n S(q)$, where f_n is the form factor, $S(q)$ is the on-shell propagator for the neutron or one of its excited states, and $\mathcal{O}_n$ is the operator corresponding to the induced vertex.

Returning to the issue of chiral transformations, we can now consider the effect of such a mapping on the the double pole contribution on the phenomenological side of the sum rule. If we consider both electric and magnetic dipole moments, then the double pole term will have the form

$$\frac{P}{2(q^2 - m_n^2)^2} \equiv \frac{1}{2(q^2 - m_n^2)^2}(\slashed{q} + m_n)(\mu F\sigma - d\tilde{F}\sigma)(\slashed{q} + m_n). \tag{8}$$

in which we have introduced the dual field strength, $\tilde{F}_{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\sigma\rho}F^{\sigma\rho}$. Under a chiral rotation, we find that the numerator P transforms as follows

$$\begin{aligned} U_\alpha P U_\alpha &= m_n\{\slashed{q}, \mu F\sigma - d\tilde{F}\sigma\} + m_n^2(\mu F\sigma - (d + \alpha\mu)(\tilde{F}\sigma)) \\ &\quad q^2(\mu F\sigma - (d - \alpha\mu)(\tilde{F}\sigma)) + 4q_\mu q_\nu \sigma_{\nu\lambda}(\mu F_{\mu\nu} - (d - \alpha\mu)\tilde{F}_{\mu\nu}), \end{aligned} \tag{9}$$
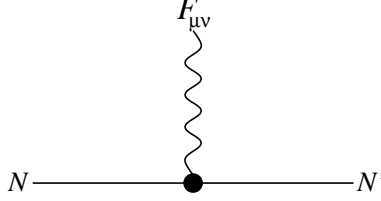
FIG. 1: Hadronic contributions to the current correlator in an external electromagnetic field. Possible excited states with the neutron quantum numbers are denoted generically by N'.

where we have retained only the zeroth and first order terms of the expansion in α, and also neglected contributions proportional to αd. We see that only Lorentz structures with an odd number of γ-matrices are independent of α. In calculating d_n, it is then clear that we should study the operator $\{\tilde{F}\sigma, \not{q}\}$, as this is the unique choice with an unambiguous coefficient.

The phenomenological side of the sum rule will therefore be parametrised in the form

$$\Pi^{(phen)} = \frac{1}{2}f(q^2)\{\tilde{F}\sigma, \not{q}\} + \cdots, \tag{10}$$

where, since we work outside the dispersion relation we may add polynomials in q^2 to ensure transversality in the chiral limit, and optimum behaviour for large q^2. We then find that the function $f(q^2)$ takes the usual form,

$$f(q^2) = \frac{\lambda^2 d_n m_n}{(q^2 - m_n^2)^2} + \sum_i \frac{f_i}{(q^2 - m_n^2)(q^2 - m_i^2)} + \sum_{i,j} \frac{f_{ij}}{(q^2 - m_i^2)(q^2 - m_j^2)}, \tag{11}$$

where λ is the coupling of the current to the neutron state (7), d_n is the neutron EDM, and f_i and f_{ij} correspond respectively to transitions between the neutron and excited states, and between the excited states themselves.

To suppress the contribution of excited states, we apply a Borel transform to Π, which we define, following [27, 28], as

$$\mathcal{B}\Pi \equiv \lim_{s,n\to\infty,s/n=M^2} \frac{s^n}{(n-1)!}\left(-\frac{d}{ds}\right)^n \Pi(s), \tag{12}$$

where $s = -q^2$. The continuum contributions in (11) are then exponentially suppressed by a factor corresponding to the gap between m_n^2 and the next excited state, usually taken around $(1.5\text{GeV})^2$. However, while this suppression is quite large, previous studies of CP-even sum rules have found that the continuum contribution is not negligible (see e.g. [28]), and it is usually included for this reason. However, when studying correlators in background fields, as mentioned above, one is effectively dealing with a three-point function and one consequently loses positivity constraints for the contributions. Thus the couplings f_{ij} for example are not sign–definite (as would be the case for the two-point function). For this reason it seems inconsistent to parametrise the continuum in the normal way, and we have no alternative but to neglect it. In practice, we shall find that the sum rule we obtain is stable in any case.

The coefficients of the single pole terms f_i are also ambiguous in sign for the same reason, but these contributions are not exponentially suppressed by the Borel transform, and must
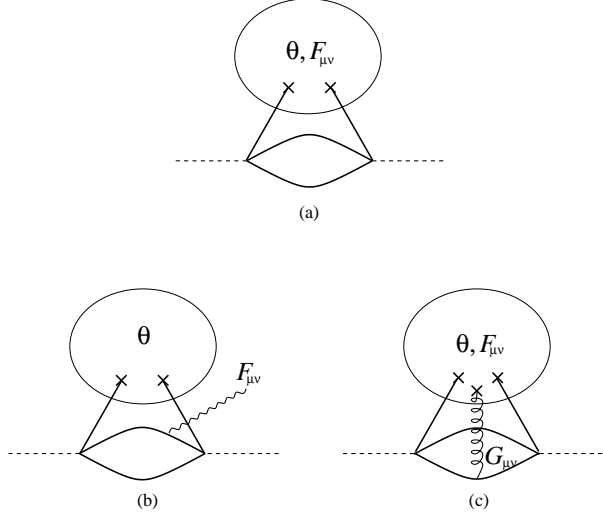
FIG. 2: Various contributions to the CP-odd structure $\{\tilde{F}\sigma, \not{q}\}$. (a) is the leading order contribution while (b) and (c) contribute at subleading order.

be included for consistency. We then find that the phenomenological expression takes the form

$$\Pi^{(phen)} = \frac{1}{2}\{\tilde{F}\sigma, \not{q}\}\left(\frac{\lambda^2 d_n m_n}{(q^2 - m_n^2)^2} + \frac{A}{q^2 - m_n^2} + \cdots\right), \tag{13}$$

where the constant A parametrizes all the single pole contributions and, as we have explained, is not sign definite. It is this expression that we shall contrast with the OPE calculation to be presented in the next section.

III. CALCULATION OF THE WILSON OPE COEFFICIENTS

We now turn to a tree-level calculation of Π (6) within the framework of the operator product expansion. The neutron interpolating current η_n is conveniently parametrised in the form,

$$\eta_n = j_1 + \beta j_2, \tag{14}$$

where the two contributions are given by

$$j_1 = 2\epsilon_{abc}(d_a^T C\gamma_5 u_b)d_c \tag{15}$$

$$j_2 = 2\epsilon_{abc}(d_a^T C u_b)\gamma_5 d_c. \tag{16}$$

The current j_2 vanishes in the nonrelativistic limit, and lattice simulations have shown that j_1 indeed provides the dominant projection onto the neutron [29] (see also [30]). From (7), we may define the coupling to the neutron state in the form $\langle 0|\eta_n|N\rangle = (\lambda_1 + \beta\lambda_2)v$, where $\lambda_2 \ll \lambda_1$.

Physical observables are independent of the parameter β, and in principle any combination of currents with neutron quantum numbers is appropriate. However, within the sum rules formalism, one has the imperative of suppressing the contribution of excited states and

higher dimensional operators in the OPE, and thus its convenient to choose β to this end. Ioffe has argued [31, 32, 33] that $\beta \sim -1$ is an apparently optimal choice from analysis of the the mass sum rule (see also [29]). An argument based on minimal sensitivity [34] leads instead to $\beta \sim -0.2$ using the same sum rule. We shall return to this issue again later, but for the moment it will be convenient to keep β arbitrary, and optimize once we have knowledge of the structure of the sum rule.

In the absence of CP violation, j_1 and j_2 form a basis for projection onto the neutron state. However, the presence of a CP violating source means that, in principle, it's also necessary to consider mixing with a CP-conjugate set of currents, which we shall write as follows,

$$i_1 = 2\epsilon_{abc}(d_a^T C u_b)d_c \tag{17}$$

$$i_2 = 2\epsilon_{abc}(d_a^T \gamma_5 C u_b)\gamma_5 d_c. \tag{18}$$

However, we shall show subsequently that it's actually possible to choose a basis for θ in which these two sets of currents do not mix, and the currents (j_1, j_2) are a diagonalised combination for projection onto the neutron state. Thus for the time being we shall focus on η_n as the full current for calculation of Π.

We now proceed to study the OPE associated with (6). The relevant diagrams we need to consider are shown in Fig. 2 ((a), (b) and (c)). In parametrizing θ, we shall take a general initial condition in which a chiral rotation has been used to generate a γ_5–mass, so that

$$\mathcal{L} \sim \cdots - \theta_q m_* \sum_f \overline{q}_f i \gamma_5 q_f + \theta_G \frac{\alpha_s}{8\pi} G_{\mu\nu}^a \tilde{G}_{\mu\nu}^a + \cdots, \tag{19}$$

in which we restrict to $q_f = u, d$, and so the reduced mass, which plays an important role in CP-odd observables, has the form,

$$m_* = \frac{m_u m_d}{m_u + m_d}. \tag{20}$$

The physical θ–parameter is of course $\overline{\theta} = \theta_q + \theta_G$, but we shall keep the general form (19) and calculate the OPE as a function of *both* phases. The independence of the final answer from $\theta_q - \theta_G$ will provide a nontrivial check on the consistency of our approach. We shall find that this requires the consideration of mixing with the additional currents (i_1, i_2), a point we shall come to shortly.

A. Leading Order Contribution

The leading order contribution is determined by the 1-loop diagram in Fig. 2(a). We work as usual with a constant background electromagnetic field, so that $A_\mu(x) = -\frac{1}{2}F_{\mu\nu}(0)x^\nu$, and for later reference we also use a fixed point gauge [35] for the gluon potential, $A_\mu^a t^a(x) = -\frac{1}{2}G_{\mu\nu}^a(0)t^a x^\nu$. At leading order it is not necessary to expand the quark propagator in the background field, but it is necessary to consider the short distance expansion of the quark wavefunction,

$$q(x) = q(0) + x_\alpha D_\alpha q(0) + \cdots, \tag{21}$$

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where $D_\alpha = \partial_\alpha - ieA_\alpha$ is the covariant derivative in the background field. When sandwiched between vacuum states, the second term contributes at first order in the quark mass via use of the equation of motion, $\not{D}q = -imq$.

The vacuum structure is conveniently encoded in a generalized propagator which incorporates the associated condensates. Projections onto particular vacuum condensates are chosen in order to obtain the Lorentz structure of interest (see e.g. [24] for more details in the present context). The electromagnetic field dependence is determined in terms of the magnetic susceptibilities χ, κ and ξ, introduced in [21]:

$$
\begin{aligned}
\langle 0|\overline{q}\sigma_{\mu\nu}q|0\rangle_F &= \chi_q F_{\mu\nu}\langle 0|\overline{q}q|0\rangle \\
g\langle 0|\overline{q}(G^a_{\lambda\sigma}t^a)q|0\rangle_F &= \kappa_q F_{\mu\nu}\langle 0|\overline{q}q|0\rangle \\
2g\langle 0|\overline{q}\gamma_5(\tilde{G}^a_{\lambda\sigma}t^a)q|0\rangle_F &= i\xi_q F_{\mu\nu}\langle 0|\overline{q}q|0\rangle,
\end{aligned}
\tag{22}
$$

while the θ–dependence is either explicit in the case of θ_q, or extracted via use of the anomalous Ward identity (see e.g. [18]) in the case of θ_G. This use of the anomalous Ward identity was discussed for example in [24], and here we simply recall that the resulting expression for a generic structure $m_q\langle\overline{q}\Gamma q\rangle_{\theta_G}$ has the form,

$$
m_q\langle 0|\overline{q}\Gamma q|0\rangle_{\theta_G} = im_*\theta_G\langle 0|\overline{q}\Gamma\gamma_5 q|0\rangle + O(m_q^2),
\tag{23}
$$

where the ability to neglect the $O(m_q^2)$ corrections follows since $m_\eta \gg m_\pi$. The overall factor has the form $(1 - m_\pi^2/m_\eta^2)$ [18] which vanishes when $U(1)$-symmetry is restored ($m_\eta \to m_\pi$) [24]. Making use of the anomaly, we see that the result then has formally the same form as arises from the θ_q γ_5–mass contribution. This is once again a consequence of the anomaly, but an important point is that the sign of these contributions may differ, and thus we may obtain contributions having the unphysical form $\theta_G - \theta_q$. The resolution of this puzzle will be described shortly.

Defining $iS(q) \equiv \langle 0|q_a(x)\overline{q}_b(0)|0\rangle_{F,\theta}$, and ignoring a trivial δ–function over colour indices, the leading order propagator adapted to the CP-odd sector and appropriate for Fig. 2(a), then takes the form,

$$
\begin{aligned}
S_{LO}(x) &= \frac{\not{x}_{ab}}{2\pi^2 x^4} + \frac{im_*}{4\pi^2 x^2}(1 - i\theta_q\gamma_5)_{ab} \\
&\quad - \frac{\chi_q m_*\overline{\theta}}{24}\langle\overline{q}q\rangle F_{\alpha\beta}x_\alpha(\gamma_\beta\gamma_5)_{ba} + \frac{i\chi_q}{24}\langle\overline{q}q\rangle(F\sigma(1 + i\theta_G\gamma_5))_{ba},
\end{aligned}
\tag{24}
$$

We shall henceforth follow [21] and assume that $\chi_q = \chi e_q$ etc., with flavour independent parameters χ, κ, ξ.

Substituting the generalized propagator into (6) according to the allowed contractions, performing the rather lengthy but straightforward algebraic manipulations, and Fourier transforming to momentum space, we find the result,

$$
\Pi_{LO}(q^2) = -\frac{\chi m_*}{64\pi^2}\langle\overline{q}q\rangle\{\tilde{F}\sigma, \not{q}\}\left[\overline{\theta}(\beta + 1)^2(4e_d - e_u) + \tilde{\theta}(1 - \beta^2)(2e_d - e_u)\right]\ln\frac{\Lambda^2}{-q^2},
\tag{25}
$$

where $\overline{\theta} = \theta_q + \theta_G$, and $\tilde{\theta} = \theta_G - \theta_q$ is an unphysical combination. The appearance of this unphysical combination is somewhat surprising and, as one might anticipate, is due to an additional source of mixing. The additional currents one needs to consider are precisely the CP conjugate set (i_1, i_2) introduced earlier on.

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In order to illustrate the effect of this mixing we shall consider first the OPE for the two-point functions

$$\langle 0|T\{j_1, \bar{j}_1\}|0\rangle, \ \langle 0|T\{i_1, \bar{i}_1\}|0\rangle, \ \langle 0|T\{j_1, \bar{i}_1\}|0\rangle, \ \langle 0|T\{i_1, \bar{j}_1\}|0\rangle. \tag{26}$$

and the Lorentz structure proportional to $\not{q}$. When both phases are set to zero, $\theta_G = \theta_q = 0$, only the diagonal, ii and jj, two-point functions survive and the cross–terms in (26) are identically zero. When the θ-phases are not zero, the ij correlators no longer vanish and an explicit calculation gives,

$$i \int d^4 x e^{iq\cdot x} \langle 0|T\{j_1, \bar{i}_1\}|0\rangle = i(\theta_G - \theta_q)\frac{3}{4\pi^2}m_*\langle \bar{q}q\rangle \not{q} \ln \frac{\Lambda^2}{-q^2} \tag{27}$$

$$i \int d^4 x e^{iq\cdot x} \left(\langle 0|T\{j_1, \bar{j}_1\}|0\rangle - \langle 0|T\{i_1, \bar{i}_1\}|0\rangle\right) = \frac{3}{2\pi^2}m_*\langle \bar{q}q\rangle \not{q} \ln \frac{\Lambda^2}{-q^2}.$$

A straightforward re-diagonalization produces two "eigencurrents", $j_1 + \frac{i\tilde{\theta}}{2}i_1$ and $i_1 - \frac{i\tilde{\theta}}{2}j_1$, not mixed in the presence of θ_G and θ_q. A similar procedure can be performed for the currents j_2 and i_2. The mixing between j_1 and i_2, and j_2 and i_1, is absent even for nonzero θ_G, θ_q because these currents differ by an overall γ_5 matrix which effectively gives an anticommutator with $\not{q}$. Therefore, the generalization of the neutron interpolating current (14) can be written in the following form,

$$\eta_n = j_1 + \beta j_2 + \frac{i\tilde{\theta}}{2} (i_1 + \beta i_2) \tag{28}$$

Since the mixing between these two sets is explicitly proportional to $\theta_G - \theta_q$, it is convenient to take $\theta_q = \theta_G$ as a useful choice of basis when working with j_1 and j_2, where the mixing between $j_{1,2}$ and $i_{1,2}$, is simply absent. This situation resembles the problem in obtaining the "correct" quark mass behavior for the EDM of ρ, addressed in [24], in which one can simplify calculations by choosing $m_u = m_d$. Alternatively, one can use the generalized form for the current and observe that the presence of extra terms in (28) gives a contribution to the OPE cancelling identically the $\tilde{\theta}$–dependence of eq. (25).

The outcome, either by including the mixing terms with (i_1, i_2), or by choosing the basis $\theta_q = \theta_G$, is the same, and we find

$$\Pi_{LO}(q^2) = -\frac{\chi m_*}{64\pi^2}\langle \bar{q}q\rangle \{\tilde{F}\sigma, \not{q}\} \left[\bar{\theta}(\beta+1)^2(4e_d - e_u)\right] \ln \frac{\Lambda^2}{-q^2}, \tag{29}$$

explicitly proportional to the physical combination $\bar{\theta}$.

B. Subleading Contributions

Diagrams (b) and (c) in Fig. 2 require, in addition, the leading order expansion in the background gluon and electromagnetic fields, and S_{NLO} is consequently more involved. We concentrate first on Fig. 2(b), which actually does not provide many non-zero contributions. In addition to the leading order propagator presented in (24), the expansion in the background field leads to,

$$S^F_{NLO} = \frac{e_q}{8\pi^2}\frac{x_\alpha}{x^2}\tilde{F}_{\alpha\beta}(\gamma_\beta\gamma_5)_{ab} - \frac{im_q e_q}{32\pi^2}\ln(-x^2)(F\sigma(1 - i\theta_q\gamma_5))_{ab}$$

$$+\frac{i}{12}\langle \bar{q}q\rangle(1 + i\theta_G\gamma_5)_{ab}. \tag{30}$$

With the field strength appearing explicitly, it is not necessary to expand the quark wavefunction, thus simplifying the calculation. The resulting expression for Π actually receives no contributions from the first term of S_{NLO} as it leads to a different Lorentz structure. However, we see that since the propagator is logarithmic in the second term, the corresponding result behaves like $\ln(-x^2)/x^4$ which gives an infrared divergence in the Fourier transform to momentum space. These divergences were also observed in [21], and we cut it off at a scale μ_{IR}. Strictly, the full OPE should be independent of such a cutoff, this dependence in the coefficient being cancelled by a similar dependence in the condensates. We shall ignore this subtlety here as these logarithmic terms will not enter our final sum rule. With this caveat, the resulting contribution to the $\{\tilde{F}\sigma, \slashed{q}\}$ structure in Π has the form,

$$\Pi(Q^2)_{NLO}^{(b)} = \frac{\overline{\theta}m_*}{16\pi^2}\langle\overline{q}q\rangle\{\tilde{F}\sigma, \slashed{q}\}(\beta-1)^2 e_d\left(\ln\frac{Q^2}{\mu_{IR}^2} - 1\right)\frac{1}{Q^2}, \tag{31}$$

where we have checked that on calculating the mixing with (i_1, i_2) the unphysical dependence on $\theta_G - \theta_q$ drops out and we are left with the expression presented here.

Diagram (c) in Fig. 2 requires considerably more work, as there are several classes of contributions arising from it. Firstly, we need to expand the quark propagator in the background gluon field, which gives rise to terms analogous to those for S_{NLO}^F given above, since we make use of a fixed point gauge. Secondly, it is also possible to project such terms onto the vacuum in order to extract the leading dependence on $F_{\mu\nu}$ using (22). This requires a first order expansion of the quark wavefunction[1]. The resulting propagator, ignoring contributions which lead to other Lorentz structures, may be written in the form

$$S_{NLO}^G = S_{(1)}^G + S_{(2)}^G, \tag{32}$$

where $S_{(1)}^G$ is the expansion in the background gluon field,

$$S_{(1)}^G = \frac{g}{8\pi^2}\frac{x_\alpha}{x^2}\tilde{G}_{\alpha\beta}(\gamma_\beta\gamma_5)_{ab} - \frac{im_qg}{32\pi^2}\ln(-x^2)(G\sigma(1-i\theta_q\gamma_5))_{ab}, \tag{33}$$

while $S_{(2)}^G$ conveniently encodes the dependence on the condensates in the form,

$$G_{\alpha\beta}S_{(2)}^G = \frac{i}{32}m_*\overline{\theta}\xi_q\langle\overline{q}q\rangle x_\rho F_{\alpha\beta}(\gamma_\rho)_{ab} - \frac{i}{24}\langle\overline{q}q\rangle(i\xi_q F_{\alpha\beta}\gamma_5 + 2\kappa_q\tilde{F}_{\alpha\beta})(1+i\theta_G\gamma_5)_{ab}. \tag{34}$$

In calculating the corresponding contributions to Π, it is understood that one picks out the appropriate cross-terms in the correlator, in order to extract the leading order dependence on θ, m_* and $F_{\mu\nu}$. Infrared divergent logarithms also arise in this case from the final term in the propagator, while the other contributions actually contribute at next-to-next-to leading order, which in this case is $O(1/Q^2)$. After a lengthy calculation, we obtain the following contributions to Π,

$$\Pi(Q^2)_{NLO}^{(c)} = \frac{\overline{\theta}m_*}{64\pi^2}\langle\overline{q}q\rangle\{\tilde{F}\sigma, \slashed{q}\}\left[(\beta-1)^2 e_d(2\kappa+\xi)\left(\ln\frac{Q^2}{\mu_{IR}^2} - 1\right)\frac{1}{Q^2}\right.$$
$$\left.\frac{\xi}{2}\left((4\beta^2 - 4\beta + 2)e_d + (3\beta^2 + 2\beta + 1)e_u\right)\frac{1}{Q^2}\cdots\right], \tag{35}$$

---

[1] Note also that a second order expansion of the wavefunction, making use of the leading order propagator, would also provide contributions at subleading order, but these are combinatorially highly suppressed [21] relative to the terms we are considering, and so will be ignored.
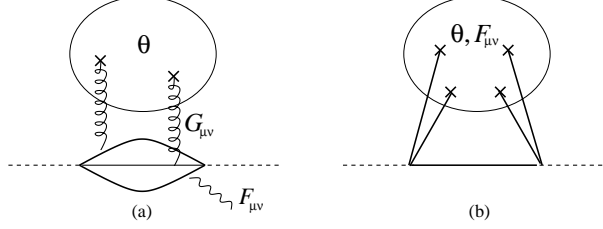
FIG. 3: Additional subleading contributions to the OPE.

where we have checked that the unphysical $\theta_G - \theta_q$ logarithmic terms are cancelled by mixing with (i_1, i_2), while we have simply used the "gauge" $\theta_G = \theta_q$ to evaluate the $O(1/Q^2)$ terms as these will turn out in fact to be numerically insignificant.

Putting all the pieces together, we present the final result for the OPE structure arising from diagrams (a), (b), and (c) in Fig. 2,

$$
\begin{aligned}
\Pi(Q^2) &= -\frac{\overline{\theta} m_*}{64\pi^2} \langle \overline{q}q \rangle \{ \tilde{F}\sigma, \not{q} \} \left[\chi(\beta+1)^2(4e_d - e_u) \ln\frac{\Lambda^2}{Q^2} \right. \\
&\quad -4(\beta-1)^2 e_d \left(1 + \frac{1}{4}(2\kappa + \xi) \right) \left(\ln\frac{Q^2}{\mu_{IR}^2} - 1 \right) \frac{1}{Q^2} \\
&\quad \left. -\frac{\xi}{2} \left((4\beta^2 - 4\beta + 2)e_d + (3\beta^2 + 2\beta + 1)e_u \right) \frac{1}{Q^2} \cdots \right].
\end{aligned}
\tag{36}
$$

This is our final result for the OPE, and we shall analyze the resulting sum rule obtained by equating this result with the phenomenological parametrization discussed in Section 2, in the next section.

However, before turning to this analysis, we shall first make some comments regarding additional contributions that we have ignored. Some additional classes of diagrams are shown in Fig. 3.

Naively, the diagram in Fig. 3(a) is loop suppressed relative to the contributions we have considered. This loop suppression is, however, fictitious as this diagram is proportional to the vacuum correlator $\alpha_s(4\pi)^{-1} \int d^4x \langle 0|(G\tilde{G}), (G\tilde{G})|0 \rangle$ which is the same as $\int d^4x \langle 0|(G\tilde{G}), m_*\overline{q}q|0 \rangle$. Nonetheless, we find in practice that all such contributions vanish.

Diagrams of the form shown in Fig. 3(b) are more problematic because they involve correlators of the form

$$
\Pi_{3(b)} \sim \int d^4x e^{iqx} \langle 0|T\{(\bar{q}q)^2(x), m_* \sum_f \overline{q}_f i\gamma_5 q_f\}|0 \rangle.
\tag{37}
$$

which are not calculable within our chiral approach. However, one suspects that these contributions of $O(\langle\overline{q}q\rangle^2)$, although suffering no loop-factor suppression, are small due in part to the small numerical size of $\langle\overline{q}q\rangle$, but also due to combinatorial factors. We estimate these contributions via saturation with the physical η meson. The result indeed turns out to be parametrically smaller than any term listed in Eq. (36).

We shall conclude this section with some brief remarks on an independent calculation of $d_n(\theta)$ using QCD sum rules, recently reported in [26]. The approach taken in this work is somewhat complementary to ours, as the authors use different Lorentz structures in (9). These structures are not chirally invariant and have an admixture of the magnetic moment

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$\alpha\mu$. Consequently, this requires simultaneous treatment of various two- and three-point correlation functions. The authors of [26] introduce a nice chirally covariant notation to assist in keeping track of these terms. In their approach, one must then try to isolate the contributions to d_n within sum rules that depend also on the neutron mass, μ, and the phase α. The subtlety here is that one must carefully keep track of all terms of $O(m_q)$, despite the fact that μ for example is determined to leading order at $O(m_q^0)$. As a result, the separation of $d \sim m\theta\langle\bar{q}q\rangle$ arises as a delicate cancelation between a combination of different terms, each of order $O(m_q^0)$. The authors of [26] simplify matters somewhat by setting all quark masses equal $m_u = m_d$, and therefore don't observe the appearance of the reduced mass m_* (20).

At first sight there is a significant problem with the use of Lorentz structures other than $\{\tilde{F}\sigma, q\!\!\!/\}$, which is the appearance at leading order of certain incalculable condensates of the form

$$\langle 0|T\{\bar{q}i\gamma_5 q(x), m_*\sum_f \bar{q}_f i\gamma_5 q_f\}|0\rangle \quad \text{and} \quad \langle 0|T\{\bar{q}\sigma_{\mu\nu}q(x), m_*\sum_f \bar{q}_f i\gamma_5 q_f\}|0\rangle. \quad (38)$$

In our approach these terms arise manifestly at $O(m_q^2)$, while for other channels these terms can arise at $O(m_q)$ and apparently need to be dealt with. The first condensate in (38) can be connected to an $O(m_*)$ correction to the correlator $\int d^4 x \langle 0|T\{\bar{q}i\gamma_5 q(x), (G\tilde{G})(0)\}|0\rangle$, for which no reliable means of extracting its value is known (for a recent discussion of the subleading mass dependence of this and related correlators see, e.g. [36]). These terms, as well as ξ and κ–proportional contributions, are ignored in [26]. However, this is consistent as one may show that, remarkably enough, in the final result for the ratio d_n/μ_n these corrections only appear at $O(m_q\langle\bar{q}q\rangle^2)$; a subleading effect. This wasn't explicitly pointed out in [26], but we believe it is an important (and indeed interesting) point, necessary for the consistency of their approach. Numerically, the results of [26] are very close to the results we obtained in [25], and shall discuss in the next section. Thus, the two approaches indeed appear quite complementary.

As a final related comment, we note that the use of chirally non-invariant channels may be the origin of numerical problems in the QCD sum rule calculations of d_n induced by color EDMs [8, 23]. This, of course, is yet to be checked but our preliminary estimates show that the use of the chirally invariant channel yields the neutron EDM at a level comparable with phenomenological estimates [10].

IV. NUMERICAL ANALYSIS OF THE SUM RULE

Turning now to the analysis of the sum rule (36), an inspection indicates that the standard choice of $\beta = -1$, appropriate for CP-even sum rules, will not be the most appropriate here as it removes the leading order contribution. In general there are two motivated criteria for fixing the mixing parameter β: (1) at a local extremum [34]; or (2) to minimize the effects of the continuum and higher dimensional operators [29, 31, 32, 33]. We find in this case that extremizing in the parameter β also leads to the unappealing cancelation of the leading order contribution. Thus the most natural procedure appears to be to choose β in order to cancel the subleading infrared logarithm which is ambiguous as a result of the required infrared cutoff. This procedure actually mimics the effect of the choice $\beta = -1$ in the sum rule for the nucleon mass. We therefore take $\beta = 1$, and it is this choice that we shall now contrast with the phenomenological side of the sum rule. It is important to note, however,

that use of the "lattice" current with $\beta = 0$ will also produce a numerically similar result. We shall make further comments on this issue at the end of the section.

On the phenomenological side of the sum rule we have (13) in which the coupling is now interpreted as $\lambda = \lambda_1 + \beta\lambda_2$. After a Borel transform of (36) and (13), and using $\beta = 1$ as discussed above, we obtain the sum rule

$$\lambda^2 m_n d_n + A M^2 = -\frac{M^4}{32\pi^2}\bar{\theta}m_*\langle\bar{q}q\rangle e^{m_n^2/M^2}$$
$$\times \left[4\chi(4e_d - e_u) - \frac{1}{2M^2}\xi(4e_d + 8e_u)\right] \qquad (39)$$

The coupling λ present in (39) may be obtained from the well known sum rules for the tensor structures $\mathbf{1}$ and $\not{q}$ in the CP even sector (see e.g. [29] for a recent review).

To aid in the presentation of the results it is convenient to define an additional function $\nu(M^2)$,

$$\nu(M^2) \equiv \frac{1}{2\bar{\theta}m_*}\left(d_n + \frac{AM^2}{\lambda^2 m_n}\right), \qquad (40)$$

which is then determined by the right hand side of (39). Inspection of (39) suggests that it is not appropriate in this case to try and remove the unknown parameter A, via differentiation for example. Instead we shall make the conventional assumption that the left hand side is a linear function of M^2 (i.e. A is independent of M^2), and construct two sum rules whose behaviour will allow us to estimate the slope of this line, and thus the parameter A. In fact this approach will lead to a result which for consistency will require $A \sim 0$, and thus allow an extraction of the EDM parameter d_n. We now construct these two sum rules as follows:

- **(a)** Firstly, we extract a numerical value for λ via a direct analysis of the CP even sum rules. This analysis has been discussed before and will not be reproduced here (see e.g. [29]). One obtains[2]

$$(2\pi)^4\lambda_a \sim 1.05 \pm 0.1, \qquad (41)$$

which leads to a sum rule of the form,

$$\nu_a(M^2) = -\frac{M^4}{64\pi^2\lambda_a^2 m_n}\langle\bar{q}q\rangle e^{m_n^2/M^2}\left[4\chi(4e_d - e_u) - \frac{1}{2M^2}\xi(4e_d + 8e_u)\right] \qquad (42)$$

- **(b)** As an alternative, we extract λ explicitly as a function of β from the CP-even sum rule for $\not{q}$ [29] which we reproduce here for completeness,

$$(2\pi)^4\lambda^2 e^{-m_n^2/M^2} = \frac{5 + 2\beta + 5\beta^2}{64}M^6\left[1 - e^{-s_1/M^2}\left(\frac{s_1^4}{2M^4} + \frac{s_1^2}{M^2} + 1\right)\right]$$
$$+ \frac{5 + 2\beta + 5\beta^2}{256}bM^2\left(1 - e^{-s_2/M^2}\right), \qquad (43)$$

---

[2] The particular choice of β in the range $[-1, 1]$ is not very important here as the numerical value for λ is not highly sensitive to this choice.
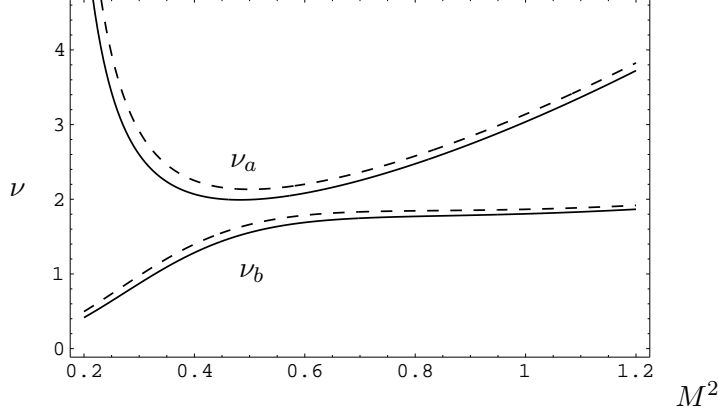
FIG. 4: The neutron EDM function $\nu(M^2(\text{GeV}^2))$ is plotted according to the sum rules (a) and (b). The dashed line shows the contribution from the leading order term only.

where s_1 and s_2 parametrise the continuum thresholds, while $b = (2\pi)^2 \langle \frac{\alpha_s}{\pi} G^2 \rangle \sim 0.47 \pm 0.2 \text{GeV}^4$, and we have neglected higher dimensional contributions, and leading-log anomalous dimension factors. The reason for the omission of the latter is that they provide a negligible contribution when M^2 is small, as will be the case here, and furthermore at this scale one has good reason to distrust the leading log approximation. Therefore, the (estimated) effect of such factors will be combined into the overall error estimate.

Solving (43) for λ_b, we obtain a new CP-odd sum rule by substituting the result into (39) and setting $\beta = 1$,

$$\nu_b(M^2) = -\frac{M^4}{64\pi^2 m_n} \langle \overline{q}q \rangle \frac{\left[4\chi(4e_d - e_u) - \frac{1}{2M^2}\xi(4e_d + 8e_u) \right]}{4M^6 c_1(M^2, s_1) + bM^2 c_2(M^2, s_2)}. \tag{44}$$

In this expression c_1 and c_2 are the continuum parametrizations introduced in (43). Throughout we shall assume $s_1 = s_2$.

We shall now proceed to analyze the sum rules numerically. Note that our assumption that $\nu(M^2)$ is linear in M^2 also requires that λ is constant in an appropriate range of the Borel parameter. This point can be checked explicitly in case (b) above.

The two sum rules described above for ν_a and ν_b are plotted in Fig. 4, where the effect of the higher dimensional terms in (39) proportional to ξ is also displayed. $\nu(M^2)$ is to be interpreted as a tangent to the curves in Fig. 4. For numerical calculation we make use of the following parameter values: For the quark condensate, we take

$$\langle 0| \overline{q}q |0 \rangle = -(0.225 \text{ GeV})^3, \tag{45}$$

while for the condensate susceptibilities, we have the values

$$\chi = -5.7 \pm 0.6 \text{ GeV}^{-2} \text{ [37]}, \tag{46}$$
$$\xi = -0.74 \pm 0.2 \text{ [23]}. \tag{47}$$

Note that χ, which enters at $O(1/M^2)$, since it is dimensionful, is numerically significantly larger than ξ. In extracting λ in case (b) we also set a relatively large continuum threshold

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$s_0 = (2\text{GeV})^2$ for consistency with the CP-odd sum rule in which this continuum is ignored for reasons discussed earlier.

One observes that both sum rules have extrema consistent to $\sim 10\%$, suggesting that our procedure for fixing the parameter β is appropriate. Furthermore, the differing behaviour away from the extrema implies that for consistency we must assume A to be small. One then finds $d_n \sim \nu(M^2 \sim 0.5\text{GeV}^2)$. It is also interesting that the effective scale is around $M \sim 0.7\text{GeV}$ which is well below m_n, and should be cause for concern regarding the convergence of the OPE. Nonetheless, one sees that the corrections associated with the leading higher dimensional operators are still quite small. This low scale is also the reason we have ignored leading-log estimates for the anomalous dimensions as noted earlier in the context of extracting the coupling λ, as their status is unclear at this scale. A naive application leads to a small correction that we shall subsume into our error estimate.

Extracting a numerical estimate for d_n from Fig. 2, and determining an approximate error arising from: (1) analysis of the sum rule; (2) the error in χ; and (3) an estimate of $\pm O(20\%)$ for higher dimensional operators and anomalous dimension factors; we find the result[3]

$$d_n = (1.0 \pm 0.4)e\overline{\theta}\frac{m_*}{(500\text{MeV})^2} = (3.6 \pm 1.4)\cdot 10^{-3}e\overline{\theta}\frac{f_\pi^2 m_\pi^2}{(100\text{MeV})^5}\frac{m_u m_d}{(m_u + m_d)^2}, \quad (48)$$

for the neutron EDM, for which the dominant contribution naturally arises from χ. Comparison with the result of Ref. [14] indicates rather good agreement in magnitude, due essentially to the low effective mass scale $M \sim 700\text{MeV}$. We also obtain d_n of the same sign if one assumes no significant corrections to the logarithm in [14] [4]. The relation between the calculation presented here and the chiral logarithm estimate will be discussed in more detail in the next section.

However, before turning to this comparison, we would like to comment further on the specific choice of the current, i.e. the choice of β. As mentioned earlier, a conventional choice for CP-even sum rules is that advocated by Ioffe [33]: $\beta = -1$. However, even in these channels, standard minimal sensitivity arguments, (as used for example in the context of renormalization scheme dependence [38]), lead instead to a choice of $\beta \sim -0.2$ [34]. Furthermore, we have found that an apparently optimal choice for the chirally invariant CP-odd channel is instead $\beta = 1$.

This variation in β might be interpreted as a sign of inherent uncertainties due to the effect of excited states or higher order condensates. However, we would like to point out that this need not be the case if these differences are observed for different physical observables, as is the case here. In particular, while one expects that the optimization of β with respect to minimizing contamination from excited states may be universal, Ioffe [33] has emphasized that this aim conflicts with the need to minimize the uncertainties due to higher dimensional operators. The latter point is quite "observable dependent", and thus the best compromise choice for β may differ for different observables. In particular, as pointed out in [29], the points $\beta \sim -1$ and $+1$ are not distinguished purely on the basis of removing contamination by excited states.

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[3] (04/2005) v4: This updated expression corrects an overall factor of two error in previous versions.

[4] The sign of $d_n(\theta)$ in [6] differs simply because of an overall minus sign in the initial definition of the θ–term.

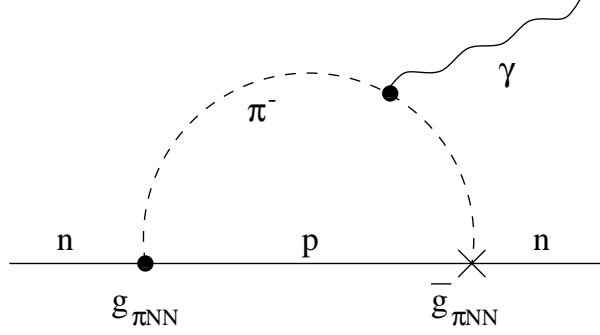FIG. 5: Leading contribution as $m_\pi \to 0$ to d_n in the chiral loop approach [14]. There is also a second diagram with the pion-nucleon vertices interchanged.

While we find such arguments for the overall consistency of the current with $\beta = 1$ compelling enough, we have also explicitly tested the β–dependence of our result. To do this, it is necessary to consider the effect of the logarithmic terms in (36). Cutting the logs at $\mu_{IR} \sim \Lambda_{QCD}$, we then find that the numerical value for d_n does not vary that dramatically with β. Indeed for $\beta \sim 0$, we find a result which is numerically within $\sim 30\%$ of the result obtained at $\beta = 1$.

V. RELATION WITH ESTIMATES FROM CHIRAL PERTURBATION THEORY

In this section, we shall consider the relation between the value for d_n we have extracted using QCD sum rules, and the well known chiral loop calculation [14]. Within the sum rules approach, use of the chiral anomaly made it quite explicit that the result would necessarily vanish in the limit $m_\eta \to m_\pi$. To compare this with the chiral result, we first need to observe how the latter also satisfies this necessary consistency condition. As far as we are aware, this result has not appeared in the literature and we present a derivation of the expected prefactor $(1 - m_\pi^2/m_\eta^2)$ in the next subsection.

Prior to addressing this issue, we first recall the main points of the chiral approach used in [14]. A chiral rotation is used to recast the θ–term into a CP violating quark mass, $\delta\mathcal{L}_{CP} = i\theta m_* \sum_f \bar{q}_f \gamma_5 q_f$. This induces an effective CP-odd interaction of pions with nucleons in terms of a small correction to the standard γ_5-interaction,

$$\mathcal{L}_{\pi NN} = \pi^a \bar{N} \tau^a (i g_{\pi NN} \gamma_5 + \bar{g}_{\pi NN}) N. \tag{49}$$

The CP-odd pion-nucleon coupling $\bar{g}_{\pi NN}$ induced by θ may be obtained by the PCAC reduction of the pion

$$\bar{g}_{\pi NN} \bar{N} \tau^a N = -\frac{i}{2 f_\pi} \langle N | [\delta\mathcal{L}_{CP}, \bar{q}\tau_a q] | N \rangle = \frac{\theta m_*}{f_\pi} \langle N | \bar{q}\tau^a q | N \rangle. \tag{50}$$

The remaining matrix element can then be expressed in terms of the mass splittings in the baryon octet using $SU(3)$ flavour symmetry. Note that the expression (50) is valid only for soft pions with momenta smaller than the characteristic hadronic scale of 1 GeV.

The crucial observation made in [14] is that the electric dipole moment of the neutron, induced by the source $\delta\mathcal{L}_{CP}$, can be estimated using the singular behaviour of the chiral
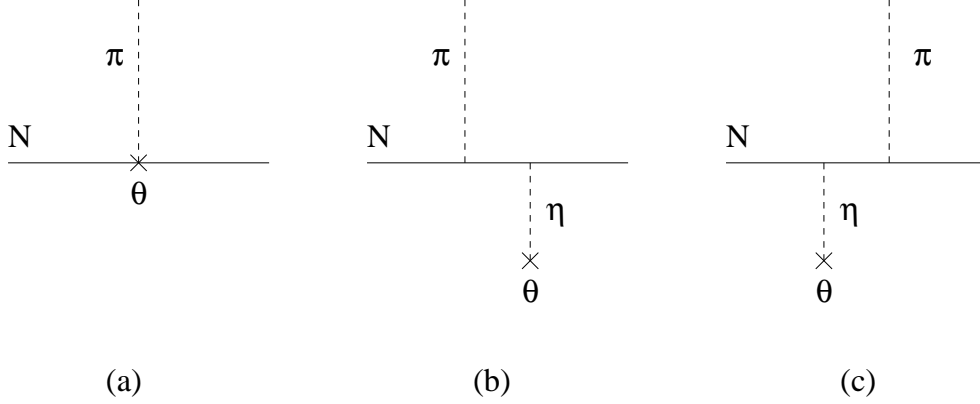
FIG. 6: Different contributions to the $\bar{g}_{\pi NN}$ coupling. The leading diagram (a) is identically cancelled by (b) and (c) in the limit $m_\eta \to m_\pi$.

loop shown in Fig. 5. The loop integral has a logarithmic infrared divergence as $m_\pi \to 0$ and one then obtains the estimate [14]

$$d_n^{\text{cpt}} = e g_{\pi NN} \bar{g}_{\pi NN} \frac{1}{4\pi^2 m_N} \ln \frac{\Lambda}{m_\pi},$$ (51)

where the cutoff represents the scale at which chiral perturbation theory breaks down. It is reasonable to assume that $\Lambda \sim m_\rho$ or m_n. After substituting the numerical expression for $\bar{g}_{\pi NN}$ we arrive at the result reproduced in (3).

A. $U_A(1)$-properties of the EDM in chiral loop calculations

The independence of the original chiral loop result (51) from m_η has been the source of some controversy, and continued work, in the literature (see e.g. [39]). Before we compare our results with that of Ref [14], we wish to point out the particular mechanism, ignored in the discussion above, which sets the EDM to zero when $U_A(1)$ symmetry is restored. This cancelation should, of course, be very similar to the vanishing of the CP-odd amplitude for $\eta \to \pi\pi$, demonstrated in [18].

Within the chiral loop approach reviewed above, the EDM depends explicitly on the CP-odd pion–nucleon coupling $\bar{g}_{\pi NN}$ induced by θ. We shall now prove that this coupling is proportional to the factor $(1 - m_\pi^2/m_\eta^2)$ for the case of two flavors, taking $m_u = m_d \equiv m_q$ for simplicity.

Recall that in the calculation of [14], the θ–term is written in the form of a singlet combination of quark γ_5–mass terms. Since the η–meson has the same quantum numbers, this combination can produce η from vacuum with an amplitude proportional to $f_\pi^{-1} m_q \langle 0|\bar{q}q|0\rangle$. Thus, the calculation of $\bar{g}_{\pi NN}$ should account for the additional contributions related to η being produced from the vacuum and then reabsorbed by the nucleon, subsequently producing the soft pion (see Fig 6).

In the absence of any physical effect from the anomaly, the mass of η should vanish in the chiral limit. In this case the flavor–singlet field η can be treated exactly as a pion field. Therefore, the amplitude for the low energy scattering $\pi N \to \eta N$ can be related to the nucleon sigma term in the triplet channel,

$$M_{\pi^a N \to \eta N} \sim m_q \langle N|\bar{q}\tau^a q|N\rangle,$$ (52)

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which is exactly the structure appearing in the calculation of the CP-odd pion–nucleon coupling constant $\bar{g}_{\pi NN}$, eq. (50).

Summing different contributions we obtain

$$\bar{g}_{\pi NN}\bar{N}\tau^a N = \frac{\theta m_q}{2f_\pi}\langle N|\bar{q}\tau^a q|N\rangle\left(1 - \frac{1}{f_\pi^2}\frac{2m_q\langle\bar{q}q\rangle}{m_\eta^2}\right) = \frac{\theta m_q}{2f_\pi}\langle N|\bar{q}\tau^a q|N\rangle\left(1 - \frac{m_\pi^2}{m_\eta^2}\right), \quad (53)$$

with the anticipated dependence on m_η^2.

Now the connection to the $U_A(1)$ problem and the vanishing of $\bar{g}_{\pi NN}$ in the limit $m_\eta \to m_\pi$ become explicit. In real life, due to the physical effect of the anomaly, m_η remains finite in the chiral limit, whereas $m_\pi \to 0$, and the correction from diagrams (b) and (c) is negligible as it is second order in the light quark masses. Thus numerical extraction of bounds on θ using this result, as in [14], are essentially unaffected by this correction. Nevertheless we find this exercise rather instructive, noting that the coupling $\bar{g}_{\pi NN}(\theta)$ may also be used for the extraction of the limit on θ from the mercury EDM experiment [3].

As a small digression, it is also worth pointing out that in [39], where the issue of $U_A(1)$ restoration was also addressed, it was suggested that contributions to $d_n(\theta)$ can be obtained within the chiral approach which are directly proportional to the anomalous magnetic moment of neutron. This seems highly unlikely since μ and d are generated at quite different energy scales. The one-loop diagram contributing to d receives contributions from momentum scales $m_\pi^2 \ll p^2 \ll 1\text{GeV}^2$, whereas similar diagrams for μ diverge quadratically and thus are saturated by momenta ~ 1 GeV where the chiral description breaks down.

B.   Relation With the EDM From Chiral Perturbation Theory

Given the numerical similarity between the result we have obtained for $d_n(\theta)$ and the estimates based on the dominance of the chiral logarithm, $\ln m_\pi$, it is natural to ask whether or not this logarithm is hidden somewhere in the OPE analysis.

Such a suggestion is necessarily speculative, as the calculations are performed using different dynamical degrees of freedom, and are in principle valid at quite different external momentum scales. Nonetheless, at first sight, one may be tempted to identify the chiral log term explicitly with the subleading infrared log–terms obtained in (36). The full momentum dependence of this term is, however, $\ln(Q^2/\mu^2)/Q^2$, and thus the singular behaviour is instead determined by $1/Q^2$. Nevertheless, one might suggest that this naive extrapolation to the chiral regime is not appropriate, and the power-like term gets softened, while the logarithm remains. The most obvious log–term of this kind arises from diagram (b) in Fig. 2. Assuming the top two quark lines are soft, as appropriate for the condensate, we can interpret this as a soft pion, and by adding two spectator quarks, we get something analogous to the chiral loop diagram contributing in the approach of [14]. Here, CP–violation arises from a particular 4-fermion vertex proportional to θ.

While such heuristic relations are sometimes possible when the momentum dependence is easily equated on both sides, we would now like to argue that, at least at large N_c, the chiral logarithm is actually subleading with respect to the leading order term in the OPE. While this need not be important numerically for $N_c = 3$, it provides a convenient parametric distinction between the results obtained using sum rules and chiral perturbation theory.

At large N_c, the $U_A(1)$ restoration factor for the chiral expression derived in the previous subsection becomes important. In particular, as is clear from the discussion above, the result

of calculation, either with the use of chiral techniques or QCD sum rules, is proportional to $(1 - m_\pi^2/m_\eta^2)$, and thus the EDM has a natural parametric dependence on θ of the form θ/N_c.

However, the main distinction between the sum rules and chiral loop calculations is that the quark diagrams used within the sum rules calculation are effectively tree-level. Thus one expects the effect to be parametrically enhanced relative to the chiral loop. Indeed, this follows from an additional suppression factor of $1/f_\pi^2$, which is $O(1/N_c)$, and which is absent in the OPE calculation. The corresponding factor has the form $\langle \bar{q}q \rangle/m_n$, which is $O(N_c/N_c \sim 1)$. Summarizing, we obtain the following behaviour at large N_c in these two cases,

$$
\begin{aligned}
\text{QCD-SR} \quad & d_n \; \propto \; \frac{\theta}{N_c} \frac{\langle 0 | \bar{q}q | 0 \rangle}{m_n} \sim O(\theta/N_c) \\
\text{Chiral Loop} \quad & d_n \; \propto \; \frac{\theta}{N_c} \frac{\langle N | \bar{u}u - \bar{d}d | N \rangle}{f_\pi^2} \sim O(\theta/N_c^2)
\end{aligned}
\tag{54}
$$

where we have only kept track of the relative N_c–dependent factors[5] It is interesting to note that the isovector matrix element $\langle N | \bar{u}u - \bar{d}d | N \rangle$ contributing to the chiral result does not grow with N_c, whereas both $\langle N | \bar{u}u | N \rangle$ and $\langle N | \bar{d}d | N \rangle$ are proportional to N_c. This is because the neutron in the large N_c limit has $(N_c - 1)/2$ u-quarks and $(N_c + 1)/2$ d-quarks.

In summary, while there appears to be at least a qualitative mechanism for mapping some of the OPE diagrams to those which would produce a chiral logarithm, the behaviour at large N_c is of the form $(c + \ln m_\pi/N_c)$. Of course, we reiterate that physically there need be no suppression for $N_c = 3$.

VI. DISCUSSION

The calculation of $d_n(\theta)$ via QCD sum rules has produced a numerical result very close to the estimates obtained using different techniques. Indeed the chiral loop estimate, QCD sum rule calculations, and even the naive quark model [13], all agree and predict essentially the same EDM to within a factor of 2-3. It is interesting to note that the power counting procedure in the chiral theory, combined with the quark model for nucleons known as naive dimensional analysis [41], also produces a similar estimate.

The situation is apparently very different in the case of dimension 5 and 6 CP-odd operators, especially for color EDMs. Different methods produce results varying within more than one order of magnitude. Moreover, none of the existing calculations is capable of answering the question of which combination of color EDMs of u, d and s quarks in fact enters into the single observable d_n. We believe that the approach developed in this paper can be used for the calculation of the neutron EDM induced by these dimension 5 and 6 CP-odd operators, and such a calculation will clarify this issue. A technical outcome of the work presented here is that the analysis can be done in the chirally invariant channel, where the OPE is directly proportional to the electric dipole moment.

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[5] An additional N_c enhancement, due to the scaling of $g_A \sim N_c$ has been discussed in relation to Skyrme model calculations (see e.g. [40]). This effect should be generic to both approaches, and we have ignored such overall contributions.

There is an additional incentive for using QCD sum rules for the calculation of d_n, as opposed to any other method. In the case of dim=5 operators, QCD sum rules would normally produce d_n in the form of a linear combination of terms like $d_q\langle\bar{q}q\rangle$, where d_q is an EDM or a color EDM of a light quark. In many models, including the MSSM and variants thereof, $d_q \sim m_q$ which would allow the removal of much of the uncertainty related to the imprecise knowledge of light quark masses. Indeed, when multiplied by the value of the quark condensate, any linear combination of d_q can be expressed in terms of $m_\pi^2 f_\pi^2$ times a function depending only on the ratio of light quark masses. The latter is known to much better accuracy than the quark masses themselves and does not depend on the normalization scale.

In conclusion, we have presented a QCD sum rules calculation of the θ-induced neutron EDM. This result is explicitly tied to a set of vacuum correlators which are non-vanishing only in the absence of a U(1) "Goldstone boson". The use of QCD sum rules in the chirally invariant channel allowed us to unambiguously extract $d_n(\theta)$, and independence of the answer from any particular representation of the theta term (19) was checked explicitly.

Combining our result with the recently improved experimental bound on d_n [2] we derive the limit on theta:

$$|\bar{\theta}| < 3 \times 10^{-10}, \tag{55}$$

which is quite close to previous bounds, and actually somewhat less constraining as our result for $d_n(\theta)$ is slightly lower than the corresponding result obtained within chiral perturbation theory with the cutoff at m_ρ. Numerically, to a large extent, our result is proportional to χ, the electromagnetic susceptibility of the vacuum.

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